

# Sparse approximation of multilinear problems with applications to kernel-based methods in UQ

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## Abstract

We provide a framework for the sparse approximation of multilinear problems and show that several problems in uncertainty quantification fit within this framework. In these problems, the value of a multilinear map has to be approximated using approximations of different accuracy and computational work of the arguments of this map. We propose and analyze a generalized version of Smolyak's algorithm, which provides sparse approximation formulas with convergence rates that mitigate the curse of dimension that appears in multilinear approximation problems with a large number of arguments. We apply the general framework to response surface approximation and optimization under uncertainty for parametric partial differential equations using kernel-based approximation. The theoretical results are supplemented by numerical experiments.

**Keywords** Multivariate approximation, Smolyak algorithm, Uncertainty quantification, Parametric PDEs, Sparse grids, Multilevel methods, Stochastic collocation methods, Kernel-based approximation

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## 1 Introduction

In the first part of this work, we consider the problem of approximating the value

$$v := \mathcal{M}(w^{(1)}, \dots, w^{(n)})$$

of a continuous multilinear map  $\mathcal{M}$ , given approximations  $w_N^{(j)}$ ,  $N \geq 0$  of the inputs  $w^{(j)}$  for  $j \in \{1, \dots, n\}$ . We assume that as  $N$  grows, the accuracy of the approximations  $w_N^{(j)}$  increases but that simultaneously the required work goes to infinity.

In practice, the map  $\mathcal{M}$  may be as simple as the application of a linear operator to a real-valued function on a domain  $\Gamma \subset \mathbb{R}^d \rightarrow \mathbb{R}$ . For example, approximating the identity operator  $w^{(1)} := \text{Id}$  by an interpolation operator based on evaluations in  $X \subset \Gamma$  with  $|X| = N$ , and approximating a function  $w^{(2)} := f$  by  $f_M: \Gamma \rightarrow \mathbb{R}$  with  $f_M \xrightarrow{M \rightarrow \infty} f$ , yields an approximation of  $v := f = \text{Id} f =: \mathcal{M}(\text{Id}, f)$  that is based on  $N$  samples of  $f_M$ . For this approximation to be accurate we need both a large number  $N$  of samples and a large  $M$  such that  $f_M$  is close to  $f$ .

In general, a straightforward approach to estimate  $v$  is to consider

$$v_N := \mathcal{M}(w_N^{(1)}, \dots, w_N^{(n)}),$$

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and let  $N \rightarrow \infty$ . If

$$\|w^{(j)} - w_N^{(j)}\| \leq N^{-\beta}$$

for all  $j \in \{1, \dots, n\}$ , then an induction argument shows

$$\|v - v_N\| \leq CN^{-\beta}.$$

However, if the work required to evaluate  $w_N^{(j)}$ ,  $j \in \{1, \dots, n\}$ , grows like  $N^\gamma$ , and if the cost for evaluating the multilinear map is multiplicative, then the work required to form  $v_N$  is

$$\text{Work}(v_N) \approx N^{n\gamma}.$$

This is an instance of the *curse of dimensionality*: To achieve the same error in  $n$  dimensions as in 1 dimension, the work needs to be exponentiated.

Smolyak's algorithm was introduced in [30] and further studied in [33, 34, 22, 7] for the case where the multilinear map is given by the tensor product of quadrature and interpolation formulas. It allows an error of size  $\exp(-\beta L)L^{n-1}$  with work  $\exp(\gamma L)L^{n-1}$  [34, Lemma 2, Lemma 7]. This means that the work required to achieve an error of size  $\epsilon > 0$  is bounded by  $\epsilon^{-\gamma/\beta} |\log \epsilon|^{(n-1)(1+\gamma/\beta)}$ . Therefore, up to logarithmic factors and multiplicative dimension-dependent constants, the curse of dimensionality has been lifted. In this work, we extend this analysis to the case of general multilinear problems and to the case where different inputs have different convergence rates, that is where  $\beta_j$  and  $\gamma_j$  may differ with  $j \in \{1, \dots, n\}$ . One implication of our results is that the work for an error of size  $\epsilon > 0$  can further be reduced to  $\epsilon^{-\gamma_{\max}/\beta_{\max}}$  for problems in which only one input has the maximal exponent ratio  $\gamma_{\max}/\beta_{\max}$ . This generalizes results for interpolation on sparse grids from [11] to dimensions  $n > 2$  and to more general problems.

When applied to the example described above, namely  $v = \mathcal{M}(\text{Id}, f)$ , Smolyak's algorithm yields a multilevel algorithm that combines samples from different approximations of  $f$  with the general idea that more samples are taken from less expensive approximations, the exact numbers being determined by the involved work and convergence rates. A connection between multilevel methods and Smolyak's algorithm has been discussed previously in [18]; however, the analysis there and in [17] was based solely on balancing errors of the involved approximations, ignoring the associated computational work.

In the second part of this work, we show how several problems in uncertainty quantification can be cast as multilinear approximation problems and tackled using the general Smolyak algorithm. We demonstrate how multilevel [9, 32, 20, 8] and multi-index [14] methods for the approximation of expectations can be regarded as instances of Smolyak's algorithm, and we obtain novel methods for kernel-based response surface approximation and optimization under uncertainty with improved theoretically guaranteed convergence rates when compared to straightforward approaches.

We study parametric partial differential equations, i.e., problems of the form

$$P_y(u_y) = f_y, \tag{1}$$

where both the partial differential operator  $P_y$  and the right-hand side  $f_y$  depend on a parameter  $y$ , and we are interested in a possibly nonlinear real-valued quantity of interest  $Q(u_y)$ . For example, Equation (1) may model physical problems with parameters describing material properties, boundary conditions and forcing terms, and  $Q$  may be a spatial average or a point value.

For numerical computations, at least two types of approximation are required. For each given parameter  $y$ , we can only compute solutions  $u_{y,N}$  of  $u_y$  stemming from discretizations of Equation (1), with  $u_{y,N} \rightarrow u_y$  as  $N \rightarrow \infty$ . Furthermore, we can only compute such approximations for finitely many values of the parameter  $y$ . The straightforward approach to obtain small errors is to take a sufficiently large number of samples computed with a sufficiently fine discretization of Equation (1) and then use a suitable interpolation method to obtain estimates of the quantity of interest for intermediate parameter values. To improve on this approach, we treat each approximation as one factor within a multilinear approximation problem. Smolyak's algorithm then yields methods that combine many samples of coarse approximations of the PDE with fewer samples of finer approximations. When the goal is to approximate an expected value, such algorithms are

called *multilevel methods* [9, 32, 20]. If the parameter space is a finite-dimensional product domain, then one may include this structure into the multilinear approximation problem and Smolyak's algorithm coincides with the *Multi-index Stochastic Collocation Method* of [16, 15]. We extend these methods to the approximation of the full response surface, which allows among others for the computation of higher statistical moments, for application to inverse problems and for the optimization of parameters. Using the general theory for Smolyak's algorithm, we obtain convergence rates that essentially only reflect the constituent approximation with the worst convergence. For example, when the response surface is smooth enough, then approximations of the full response surface can be obtained at the same cost as response approximations for one single value of the parameter. To construct approximations of the response surface, we use kernel-based approximation [25], for which we provide the required background in Section 3. As a by-product, we obtain novel bounds for kernel-based approximation using sparse grids. Previous work in this direction [26] established convergence bounds in the  $L^\infty$ -norm; we extend these bounds to Sobolev norms and more general function spaces. We note in passing that the choice of kernel-based approximations is not crucial. Indeed, any interpolation or approximation method that provides operators converging to the identity in some appropriate operator norm may be used. The strengths of kernel-based approximation are that the domain is not restricted to be an interval or hypercube, the data can be given in an unstructured form (i.e. not on a grid), and more general types of information (e.g. derivative values) can easily be included to enhance the resulting approximation.

Finally, we consider problems where the parameter  $y = (z, m)$  of Equation (1) can be split into a deterministic part  $z \in \Gamma \subset \mathbb{R}^d$  and a random part  $m$ . For example, this gives rise to the minimization problem

$$\min_z E[Q(u_{(z,m)})] + \psi(z), \quad (2)$$

which is an instance of optimization under uncertainty [24, 28]. We show how response surface approximation for  $z$  (using kernel-based approximation), expectations over  $m$  (using Monte Carlo sampling) and numerical approximation of the PDE (using black-box PDE solvers) can be treated jointly in a multilinear approximation setting. Applying Smolyak's algorithm then gives rise to a novel method for the approximative solution of (2). More specifically, we obtain surrogate models that can be evaluated at low cost such that standard minimization procedures can be applied. Under some assumptions, these surrogate models converge to the true model at the rate of Monte Carlo methods, which means that the work required for approximation of the PDE and for interpolation between finitely many choices of the parameter becomes negligible.

The remainder of this work is organized as follows. In Section 2, we introduce multilinear approximation problems and analyze Smolyak's algorithm applied to this setting. In Section 3 we provide a short introduction to kernel-based approximation and show how mixed regularity gives rise to a multilinear structure that may be exploited using the results of Section 2, yielding kernel-based approximation with sparse grids. In Section 4, we study the numerical approximation of parametric and random PDEs. Applying the results from Section 2, we obtain novel sparse kernel-based approximation methods with theoretically guaranteed convergence rates. In Section 5, we present numerical experiments on parametric, linear elliptic PDE problems that confirm the theoretical convergence rates for response surface approximation and optimization under uncertainty.

## 2 Sparse approximation of multilinear problems

Suppose we want to approximate the value

$$v := \mathcal{M}(w^{(1)}, \dots, w^{(n)})$$

of a multilinear map

$$\mathcal{M}: W^{(1)} \times \dots \times W^{(n)} \rightarrow V,$$

where  $W^{(1)}, \dots, W^{(n)}$  and  $V$  are normed spaces, and  $w^{(j)}$  are fixed but not available inputs for which we are given approximations  $w_N^{(j)} \xrightarrow{N \rightarrow \infty} w^{(j)}$ ,  $j \in \{1, \dots, n\}$ .

In the applications that we consider in this work (see Sections 3 and 4), each input  $w^{(j)}$  will be either a real-valued function (where the need for approximation comes from the discretized

solution of differential equations that define these functions), an identity operator (which will be approximated by interpolation operators based on finitely many deterministic samples), or an expected value (which is again approximated using finitely many, either deterministic or random, samples). The multilinear map  $\mathcal{M}$  will be a combination of applications of operators to elements of their domain and of tensor products of operators. Finally, the value  $v$  will be a scalar, a real-valued function, or an operator.

A straightforward way to approximate  $v$  is to consider

$$\mathcal{M}(w_{N^{(1)}}^{(1)}, \dots, w_{N^{(n)}}^{(n)})$$

with large  $N^{(j)}$  for all  $j \in \{1, \dots, n\}$ . Under the assumptions stated below, the work required by this approach for an error of size  $\epsilon > 0$  grows like  $\epsilon^{-\gamma_1/\beta_1 - \dots - \gamma_n/\beta_n}$ . We will derive an alternative, decomposition based approximation of  $v$  that reduces the workload to  $\epsilon^{-\rho}$ ,  $\rho := \max_{j=1}^n \gamma_j/\beta_j$ , up to possible logarithmic factors. In the context of integration and interpolation problems, this approach is known as Smolyak's algorithm [30].

- **Assumption 1 (Continuity):** The map  $\mathcal{M}$  is continuous. This is equivalent to the existence of a constant  $C > 0$  such that

$$\|\mathcal{M}(a^{(1)}, \dots, a^{(n)})\| \leq C \prod_{j=1}^n \|a^{(j)}\|$$

for any  $\{a^{(j)}\}_{j=1}^n \in \prod_{j=1}^n W^{(j)}$ . Here and in the remainder of this work, we use the generic symbol  $\|\cdot\|$  to denote norms whenever it is evident from the context which specific norm is meant.

- **Assumption 2 (Componentwise approximability):** For each  $j \in \{1, \dots, n\}$ , we have

$$\|w^{(j)} - w_N^{(j)}\| \lesssim_N N^{-\beta_j}$$

for some  $\beta_j > 0$ . We use the notation  $\lesssim_N$  to denote inequalities that hold up to a factor that is *independent* of  $N$ .

- **Assumption 3 (Componentwise required work):** For each  $j \in \{1, \dots, n\}$ , the construction of  $w_N^{(j)}$  requires the work

$$\text{Work}(w_N^{(j)}) \lesssim_N N^{\gamma_j}$$

for some  $\gamma_j > 0$ .

- **Assumption 4 (Overall work):** The work required for the evaluation of  $\mathcal{M}$  is multiplicative,

$$\text{Work}(\mathcal{M}(a^{(1)}, \dots, a^{(n)})) = \prod_{j=1}^n \text{Work}(a^{(j)})$$

for any  $\{a^{(j)}\}_{j=1}^n \in \prod_{j=1}^n W^{(j)}$ , and the work is subadditive with respect to addition, that is

$$\text{Work}(v_1 + v_2) \leq \text{Work}(v_1) + \text{Work}(v_2)$$

for  $v_1, v_2 \in V$ .

To define Smolyak's algorithm, for any  $j \in \{1, \dots, n\}$  we consider subsequences  $N_l^{(j)} := \exp(t_j l)$ ,  $l \in \mathbb{N} := \{1, \dots\}$ , with  $t_j > 0$  to be chosen below, and we define the consecutive differences

$$\Delta_l^{(j)} := w_{N_l^{(j)}}^{(j)} - w_{N_{l-1}^{(j)}}^{(j)} \quad \forall l \geq 1$$

with the auxiliary definition  $w_{N_0^{(j)}}^{(j)} := 0$ . Deferring questions of convergence to Lemma 2.2 below, we can write

$$\begin{aligned}
v &= \mathcal{M}(w^{(1)}, \dots, w^{(n)}) \\
&= \mathcal{M}\left(\sum_{l_1=1}^{\infty} \Delta_{l_1}^{(1)}, \dots, \sum_{l_n=1}^{\infty} \Delta_{l_n}^{(n)}\right) \\
&= \sum_{\mathbf{l} \in \mathbb{N}^n} \mathcal{M}(\Delta_{l_1}^{(1)}, \dots, \Delta_{l_n}^{(n)}) \\
&=: \sum_{\mathbf{l} \in \mathbb{N}^n} \Delta_{\mathbf{l}}.
\end{aligned} \tag{3}$$

It is now reasonable to restrict the final sum in the above decomposition of  $v$  to those multi-indices  $\mathbf{l} \in \mathbb{N}^n$  for which the ratio of work and contribution (measured by the norm) associated with

$$\Delta_{\mathbf{l}} = \mathcal{M}(\Delta_{l_1}^{(1)}, \dots, \Delta_{l_n}^{(n)})$$

is below some threshold. Thanks to Assumptions 3 and 4, the work associated with  $\Delta_{\mathbf{l}}$  can be bounded by

$$\begin{aligned}
\text{Work}(\Delta_{\mathbf{l}}) &= \prod_{j=1}^n \text{Work}(\Delta_{l_j}^{(j)}) \\
&\leq \prod_{j=1}^n [\exp(\gamma_j t_j l_j) + \exp(\gamma_j t_j (l_j - 1))] \\
&\lesssim_{\mathbf{l}} \prod_{j=1}^n \exp(\gamma_j t_j l_j)
\end{aligned} \tag{4}$$

and due to Assumptions 1 and 2, the norm of  $\Delta_{\mathbf{l}}$  can be bounded by

$$\begin{aligned}
\|\Delta_{\mathbf{l}}\| &\leq C \prod_{j=1}^n \|w_{l_j}^{(j)} - w_{l_j-1}^{(j)}\| \\
&\lesssim_{\mathbf{l}} \prod_{j=1}^n \exp(-\beta_j t_j l_j).
\end{aligned} \tag{5}$$

Therefore, we approximate the work-to-contribution ratio of  $\Delta_{\mathbf{l}}$  by

$$\exp\left(\sum_{j=1}^n (\gamma_j + \beta_j) t_j l_j\right). \tag{6}$$

Since strict inequalities in our derivations above are possible, this approximation may not be exact, and therefore merely functions as a motivation for the following definitions. Looking at (6), we may proceed in two ways. Either we choose  $t_j := 1/(\gamma_j + \beta_j)$  and restrict the sum in Equation (3) to those  $\Delta_{\mathbf{l}}$  with  $|\mathbf{l}|_1 := l_1 + \dots + l_n \leq L \in \mathbb{N}$  or we take  $t_j$  to be constant and sum up all  $\Delta_{\mathbf{l}}$  with  $(\gamma + \beta) \cdot \mathbf{l} \leq L$ . We choose the first option and define *Smolyak's algorithm*

$$\mathcal{S}_L(v) := \sum_{|\mathbf{l}|_1 \leq L} \Delta_{\mathbf{l}} = \sum_{|\mathbf{l}|_1 \leq L} \mathcal{M}(\Delta_{l_1}^{(1)}, \dots, \Delta_{l_n}^{(n)}). \tag{7}$$

(Here and in the remainder of this work, the sum only includes multi-indices for which  $\Delta_{\mathbf{l}}$  is defined, i.e.,  $\mathbf{l} \in \mathbb{N}^n$ .) This is of course simply an element of  $V$ ; the word *algorithm* is used because in Smolyak's original publication [30] the factors  $w_N^{(j)}$  were univariate interpolation or quadrature formulas, the multilinear map corresponded to the tensor product of these operators, and Smolyak's

algorithm provided instructions for the combination of the previously known univariate formulas to obtain novel corresponding multivariate formulas.

By Equation (4), the work associated to  $\mathcal{S}_L(v)$  is bounded by

$$\text{Work}(\mathcal{S}_L(v)) \leq \sum_{|\mathbf{l}|_1 \leq L} \exp(\mathbf{g} \cdot \mathbf{l}), \quad (8)$$

where  $\mathbf{g} = (g_1, \dots, g_n)$  with  $g_j := \gamma_j / (\gamma_j + \beta_j)$ . This sum has been estimated in [16, Lemma 6] with the result

$$\text{Work}(\mathcal{S}_L(v)) \lesssim_L \exp(g_{\max} L) L^{n^+(\mathbf{g})-1}, \quad (9)$$

where  $g_{\max} := \max_{j=1}^n g_j$  and  $n^+(\mathbf{g}) := |\{j : g_j = g_{\max}\}|$ . Furthermore, Equations (3) and (5) (see Lemma 2.2 below for a rigorous justification) show that

$$\|v - \mathcal{S}_L(v)\| = \left\| \sum_{|\mathbf{l}|_1 > L} \Delta_{\mathbf{l}} \right\| \lesssim_L \sum_{|\mathbf{l}|_1 > L} \exp(-\mathbf{b} \cdot \mathbf{l}), \quad (10)$$

where  $\mathbf{b} = (b_1, \dots, b_n)$  with  $b_j := \beta_j / (\gamma_j + \beta_j) = 1 - g_j$ . In this case, [16, Lemma 7] provides the estimate

$$\|v - \mathcal{S}_L(v)\| \lesssim_L \exp(-b_{\min} L) L^{n^-(\mathbf{b})-1}, \quad (11)$$

where  $b_{\min} := \min_{j=1}^n b_j$  and  $n^-(\mathbf{b}) := |\{j : b_j = b_{\min}\}|$ .

To summarize the results in a succinct fashion, we define

$$\rho := \max_{j=1}^n \gamma_j / \beta_j = g_{\max} / b_{\min}$$

and

$$n_0 := |\{j : \gamma_j / \beta_j = \rho\}| = n^-(\mathbf{b}) = n^+(\mathbf{g}).$$

**Theorem 2.1. (Convergence of sparse approximations)** *For  $\epsilon > 0$  small enough, we can choose  $L = L(\epsilon)$  such that*

$$\|\mathcal{S}_L(v) - v\| \lesssim_{\epsilon} \epsilon \quad (12)$$

and

$$\text{Work}(\mathcal{S}_L(v)) \lesssim_{\epsilon} \epsilon^{-\rho} |\log \epsilon|^{(n_0-1)(1+\rho)}. \quad (13)$$

*Proof.* Given  $\epsilon > 0$ , let  $L$  be the largest integer such that  $\psi(L) := \exp(-b_{\min} L) L^{n_0-1} > \epsilon$ . By Equation (11), and because  $\psi(L)/\psi(L+1)$  is bounded and  $\psi(L+1) \leq \epsilon$ , this implies Equation (12). Furthermore, by Equation (9) we have

$$\begin{aligned} \text{Work}(\mathcal{S}_L(v)) &\lesssim_L \exp(g_{\max} L) L^{n_0-1} \\ &= \exp(\rho b_{\min} L) L^{-(n_0-1)\rho} L^{(n_0-1)(1+\rho)} \\ &\lesssim_L \psi(L)^{-\rho} |\log \psi(L)|^{(n_0-1)(1+\rho)} \\ &\leq \epsilon^{-\rho} |\log \epsilon|^{(n_0-1)(1+\rho)}, \end{aligned}$$

where the last inequality holds for all small enough  $\epsilon > 0$  by the choice of  $L$ .  $\square$

**Remark 1. (Combination rule)** *The following combination rule [12] can be proven verbatim as in [34, Lemma 1] and facilitates numerical implementations:*

$$\mathcal{S}_L(v) = \sum_{L-n+1 \leq |\mathbf{l}|_1 \leq L} (-1)^{L-|\mathbf{l}|_1} \binom{n-1}{L-|\mathbf{l}|_1} v_{\mathbf{l}}, \quad (14)$$

where

$$v_{\mathbf{l}} := \mathcal{M}(w_{N_{t_1}^{(1)}}^{(1)}, \dots, w_{N_{t_n}^{(n)}}^{(n)}).$$

**Remark 2. (Exponential convergence)** It may happen that one of the inputs exhibits exponential convergence,

$$\|w^{(j)} - w_N^{(j)}\| \lesssim_N \exp(-s_j N)$$

and algebraic work,

$$\text{Work}(w_N^{(j)}) \lesssim_N N^{\gamma_j}.$$

Such inputs satisfy Assumption 2 for any exponent and thus can always be added to a problem without increasing the bounds in Theorem 2.1. When all inputs converge exponentially, improved exponential convergence rates can be obtained by an extended analysis, see Remark 7 and [10].

**Remark 3. (Logarithmic factors)** If the work of one of the inputs exhibits additional logarithmic factors,

$$\text{Work}(w_N^{(j)}) \lesssim_N N^{\gamma_j} (\log N)^{\mu_j},$$

then the work required for an error of size  $\epsilon$  increases by the factor  $|\log \epsilon|^s$ , where  $s := \sum_{\{j: \gamma_j/\beta_j=\rho\}} \mu_j$ . Indeed,  $\sum_{|l|_1 \leq L} \exp(\mathbf{g} \cdot \mathbf{l}) \prod_{j=1}^n l_j^{\mu_j} \lesssim_L \exp(g_{\max} L) L^{n^+(\mathbf{g})-1+s}$ , which follows from a simple supremum bound together with [16, Lemma 6]. Therefore, Equation (9) holds with the additional factor  $L^s$  and Theorem 2.1 holds with the additional factor  $|\log \epsilon|^s$ .

**Remark 4. (Explicit constants)** Provided more explicit bounds on error and work,

$$\begin{aligned} \|w^{(j)} - w_N^{(j)}\| &\leq C_{E,j} N^{-\beta_j} \\ \text{Work}(w_N^{(j)}) &\leq C_{W,j} N^{\gamma_j}, \end{aligned}$$

we may refine the work bound in Theorem 2.1 to

$$\text{Work}(\mathcal{S}_L(v)) \lesssim_{\epsilon, C_E, C_W} C_W C_E^\rho \epsilon^{-\rho} |\log \epsilon|^{(n_0-1)(1+\rho)}, \quad (15)$$

for  $C_W := \prod_{j=1}^n C_{W,j}$  and  $C_E := \prod_{j=1}^n C_{E,j}$ .

**Remark 5. (Integer constraints)** We assumed that we can choose  $N \in \mathbb{R}_{\geq} := \{x \in \mathbb{R} : x \geq 0\}$ . In practice,  $N$  is often restricted to being a natural number. If we implicitly round up all occurrences of  $N$ , then the analysis above goes through since the error bound in Equation (5) persists unaltered and the work bound in Equation (4) persists with another constant.

**Lemma 2.2.** Under Assumptions 1 and 2, the elements  $\Delta_{\mathbf{l}} \in V$  are absolutely summable and their sum is  $v$ . In particular,

$$v - \sum_{|\mathbf{l}|_1 \leq L} \Delta_{\mathbf{l}} = \sum_{|\mathbf{l}|_1 > L} \Delta_{\mathbf{l}}.$$

*Proof.* By Equation (5) and [16, Lemma 7] we have

$$\sum_{\mathbf{l} \in \mathbb{N}^d} \|\Delta_{\mathbf{l}}\| < \infty.$$

Therefore, all rearrangements yield the same limit, if one exists. But

$$\sum_{|\mathbf{l}|_{\infty} \leq L} \Delta_{\mathbf{l}} = \mathcal{M}\left(\sum_{l_1=1}^L \Delta_{l_1}^{(1)}, \dots, \sum_{l_n=1}^L \Delta_{l_n}^{(n)}\right) = \mathcal{M}(w_L^{(1)}, \dots, w_L^{(n)}) \rightarrow v$$

by continuity of  $\mathcal{M}$ . □

### 3 Kernel-based approximation

In this section, we describe kernel-based approximation methods [25, 35], which we later use to approximate response surfaces.

Assume we want to reconstruct an element  $f$  of a Hilbert space  $(H, \langle \cdot, \cdot \rangle)$  from the output  $Tf$  of a linear *sampling operator*  $T \in \mathcal{L}(H, \mathbb{R}^N)$ , with  $N \in \mathbb{N}$ .

If  $H$  is infinite-dimensional, then the output of  $T$  never uniquely determines an element of  $H$ . To resolve this ambiguity we select the interpolant with minimal norm,

$$Sf := \arg \min_{\substack{s \in H \\ Ts = Tf}} \|s\|^2, \quad (16)$$

where  $\|s\|^2 := \langle s, s \rangle$ . In the remainder of this work, we refer to  $S$  as the *best-approximation associated with  $T$* , which is justified by property (ii) in Theorem 3.1 below.

We denote by  $T^*: \mathbb{R}^N \rightarrow H$  the Hilbert space adjoint of  $T$ . For the sake of simplicity we assume that  $H$  is a real Hilbert space and that  $T$  is surjective, which is the case in all applications we consider in this work. In particular, this implies that  $T^*$  is injective and  $TT^*$  invertible.

**Theorem 3.1.** (i) *The best-approximation  $S$  from Equation (16) is well-defined, linear, and satisfies*

$$S = T^*(TT^*)^{-1}T. \quad (17)$$

(ii)  *$Sf$  is the best approximation to  $f$  from  $(\ker T)^\perp$ : For any  $f \in H$ , we have*

$$\|f - Sf\| = \inf_{g \in (\ker T)^\perp} \|f - g\|.$$

*Proof.* Equation (16) defines  $Sf$  as the minimal-norm approximation of  $f$  from the affine subspace  $f + \ker T$ . In Hilbert spaces, this coincides with the orthogonal projection, which is uniquely determined by  $TSf = Tf$  and  $\langle Sf, v \rangle = 0$  for all  $v \in \ker T$ . Both of these equations are satisfied by  $Sf = T^*(TT^*)^{-1}Tf$ , which proves (i). From here we see that  $Sf \in \text{Im } T^* = (\ker T)^\perp$  and  $f - Sf \in \ker T = ((\ker T)^\perp)^\perp$ , which implies that  $Sf$  is also the orthogonal projection of  $f$  onto  $(\ker T)^\perp$  and thus (ii) holds.  $\square$

If our objects of interest are real-valued functions on domains  $\Gamma \subset \mathbb{R}^d$ , an explicit classification of all Hilbert spaces of such functions is desirable. Under the additional assumption that point evaluations are continuous, this can be achieved through *reproducing kernels*.

**Definition 3.2.** *A Hilbert space  $(H, \|\cdot\|)$  of functions on  $\Gamma \subset \mathbb{R}^d$  such that all point evaluations  $\delta_x f := f(x)$ ,  $x \in \Gamma$  are continuous with respect to  $\|\cdot\|$  is called Reproducing Kernel Hilbert Space (RKHS). We call  $\Phi: \Gamma \times \Gamma \rightarrow \mathbb{R}$ ,  $\Phi(x, y) := \mathcal{R}(\delta_x)(y)$  the reproducing kernel of  $H$ , where  $\mathcal{R}: H^* \rightarrow H$  is the Riesz isometry.*

It can be shown [2] that the reproducing kernel of an RKHS is symmetric and positive definite on  $\Gamma \times \Gamma$ , meaning that

$$(\Phi(x_i, x_j))_{i,j=1}^N$$

is positive definite for any  $\{x_1, \dots, x_N\} \subset \Gamma$ . Conversely, any function that satisfies these conditions is the reproducing kernel of a unique RKHS, which is called the *native space* of  $\Phi$  and denoted by  $\mathcal{N}_\Phi(\Gamma)$ .

Depending on the context, the application of best-approximation theory in Hilbert spaces to the reconstruction of functions in RKHS is called kernel-based approximation [5], scattered data approximation [35], kriging [31], or kernel learning [27].

For practical applications it is crucial that, given the reproducing kernel, best-approximations can be computed exactly. The following proposition is well known in the theory of kernel-based approximation; we provide a proof for the convenience of the reader.



**Proposition 3.3.** *Let  $T = (\lambda_1, \dots, \lambda_N)$  with  $\lambda_i \in H^*$ . Then*

$$Sf = \sum_{i=1}^N s_i \lambda_i f,$$

where

$$s_i = \sum_{j=1}^n u_{ij} \lambda_j^1 \Phi \in H$$

and  $(u_{ij})_{i,j=1}^N$  are the entries of the inverse of  $(\lambda_i^2 \lambda_j^1 \Phi)_{i,j=1}^N$ . Here, the superscript indicates the variable that is acted on. For example, if  $T$  consists of point evaluations in  $\{x_1, \dots, x_N\} \subset \Gamma$ , then  $\lambda_j^1 \Phi = \Phi(x_j, \cdot) \in H$  and  $\lambda_i^2 \lambda_j^1 \Phi = \Phi(x_j, x_i) \in \mathbb{R}$ .

*Proof.* In view of Equation (17) it suffices to note that  $T^*v = \sum_{i=1}^N \lambda_i^1 \Phi v_i$  for any  $v \in \mathbb{R}^N$  and therefore  $TT^*v = (\sum_{i=1}^N (\lambda_j^2 \lambda_i^1 \Phi) v_i)_{j=1}^N$ . We have seen in Theorem 3.1 that  $TT^*$  is invertible.  $\square$

Maybe the most common examples of reproducing kernel Hilbert spaces are the isotropic Sobolev spaces  $H^\beta(\mathbb{R}^d)$  with  $\beta > d/2$ , for which point evaluations are continuous by Sobolev's embedding theorem. We give here a general definition using Fourier transforms that is suited to our interest in multilinear problems. For a partition  $D = \{D_j\}_{j=1}^n$  of  $\{1, \dots, d\}$ , with  $d_j := |D_j|$ , and  $\beta \in \mathbb{R}_{\geq}^n$ , we define

$$H_D^\beta(\mathbb{R}^d) := \{f \in L^2(\mathbb{R}^d) : \|f\|_{H_D^\beta(\mathbb{R}^d)} := \left\| \prod_{j=1}^n (1 + |\omega_{D_j}|^2)^{\beta_j/2} \hat{f} \right\|_{L^2(\mathbb{R}^d)} < \infty\},$$

equipped with the obvious inner product, where we denote by  $|\cdot|$  the Euclidean norm, and where we access groups of components of  $\omega \in \mathbb{R}^d$  by the subscripts  $D_j$ . Furthermore, for any  $\Gamma \subset \mathbb{R}^d$  we define  $H_D^\beta(\Gamma)$  as space of restrictions of functions in  $H_D^\beta(\mathbb{R}^d)$  with the norm  $\|f\|_{H_D^\beta(\Gamma)} := \inf_{g|_\Gamma = f} \|g\|_{H_D^\beta(\mathbb{R}^d)}$ .

Special cases are the isotropic Sobolev spaces, which correspond to  $D_1 = \{1, \dots, d\}$  and  $\beta = \beta \in \mathbb{R}_{\geq}$ , and the Sobolev spaces  $H_{\text{mix}}^\beta(\mathbb{R}^d)$  of dominating mixed smoothness, which correspond to  $D_j = \{j\}$  and  $\beta_j = \beta \in \mathbb{R}_{\geq}$  for  $j \in \{1, \dots, d\}$ .

If  $\beta \in \mathbb{N}_0^n$ , then we have the characterization

$$H_D^\beta(\mathbb{R}^d) := \{f \in L^2(\mathbb{R}^d) : \forall \alpha \in \mathbb{N}_0^d, |\alpha_{D_j}|_1 \leq \beta_j, j \in \{1, \dots, n\} : \|\partial_\alpha f\|_{L^2(\mathbb{R}^d)} < \infty\}.$$

Furthermore, we see below that the spaces  $H_D^\beta(\Gamma)$  are tensor products of isotropic Hilbert spaces when  $\Gamma$  is a product domain. The multilinearity of the tensor product will later allow us to apply the general framework from Section 2.

**Definition 3.4** ([13]). *If  $(H^{(j)}, \langle \cdot, \cdot \rangle_j)$  are Hilbert spaces for  $j \in \{1, \dots, n\}$ , then the unique bilinear extension of*

$$\left\langle \bigotimes_{j=1}^n f_1^{(j)}, \bigotimes_{j=1}^n f_2^{(j)} \right\rangle_H := \prod_{j=1}^n \langle f_1^{(j)}, f_2^{(j)} \rangle_j,$$

*is an inner product on their algebraic tensor product. We call the completion of the algebraic tensor product under this inner product the Hilbert tensor product and denote it  $\bigotimes_{j=1}^n H^{(j)}$ .*

**Proposition 3.5.** (i) *Let  $\{D_j\}_{j=1}^n$  be a partition of  $\{1, \dots, d\}$ . If for each  $j \in \{1, \dots, n\}$  we have a function  $\phi_j : \mathbb{R}^{d_j} \rightarrow \mathbb{R}$  that satisfies*

$$(1 + |\omega|^2)^{-\beta_j} \lesssim_\omega |\hat{\phi}_j(\omega)| \lesssim_\omega (1 + |\omega|^2)^{-\beta_j},$$

*for some  $\beta_j/2 > d_j$ , then  $\Phi(x, y) := \prod_{j=1}^n \phi_j(x_{D_j} - y_{D_j}) : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$  is a reproducing kernel with native space  $\mathcal{N}_\Phi(\mathbb{R}^d) \simeq H_D^\beta(\mathbb{R}^d)$ .*

(ii) If  $\Phi: \Lambda \times \Lambda \rightarrow \mathbb{R}$  is a reproducing kernel, and  $\Gamma \subset \Lambda$ , then  $\Phi|_{\Gamma \times \Gamma}$  is the reproducing kernel of the space of restrictions equipped with the natural norm:

$$\mathcal{N}_{\Phi|_{\Gamma \times \Gamma}}(\Gamma) = (\{g|_{\Gamma} : g \in \mathcal{N}_{\Phi}(\Lambda)\}, \|f\|_{\mathcal{N}_{\Phi}(\Gamma)} = \inf_{g|_{\Gamma}=f} \|g\|_{\mathcal{N}_{\Phi}(\Lambda)}).$$

(iii) If  $\Phi_j: \Gamma_j \times \Gamma_j \rightarrow \mathbb{R}$  are reproducing kernels for  $j \in \{1, \dots, n\}$ , then  $\Phi := \bigotimes_{j=1}^n \Phi_j$  is a reproducing kernel and  $\mathcal{N}_{\Phi}(\prod_{j=1}^n \Gamma_j) = \bigotimes_{j=1}^n \mathcal{N}_{\Phi_j}(\Gamma_j)$ .

(iv) Let  $\{D_j\}_{j=1}^n$  be a partition of  $\{1, \dots, d\}$  and assume that  $\beta_j > d_j/2$  for all  $j \in \{1, \dots, n\}$ . Then

$$H_D^{\beta}(\prod_{j=1}^n \Gamma_j) = \bigotimes_{j=1}^n H^{\beta_j}(\Gamma_j).$$

for any  $\Gamma_j \subset \mathbb{R}^{d_j}$ ,  $j \in \{1, \dots, n\}$ .

*Proof.* (i) Follows from [35, Theorem 10.12].

(ii) This is [2, Section 5, Theorem 1].

(iii) This is [2, Section 8, Theorem 1].

(iv) Follows from combining (i) through (iii). □

A family of functions that satisfy the condition in part (i) are the *Matérn functions*

$$\phi: \mathbb{R}^d \rightarrow \mathbb{R}, x \mapsto \phi(x) := \frac{2^{1-\beta}}{\Gamma(\beta)} |x|^{\beta-d/2} K_{\beta-d/2}(|x|),$$

where  $\beta > d/2$ , and  $K_{\beta-d/2}(r)$  is the modified Bessel function of the second kind of order  $\beta - d/2$ . Their Fourier transform equals  $(1 + |\omega|^2)^{-\beta}$  [35, Theorem 6.13]. By parts (ii) through (iii) of the previous proposition, we therefore have explicit expressions of the reproducing kernels of the generalized Sobolev spaces  $H_D^{\beta}(\Gamma)$ . In combination with Proposition 3.3 this allows the effective computation of best-approximations in these spaces.

Error bounds for best-approximations in isotropic Sobolev spaces can be deduced from the *sampling inequality* in Proposition 3.6 below. For subsets  $X \subset \Gamma$  we denote by

$$h_{X,\Gamma} := \sup_{y \in \Gamma} \inf_{x \in X} |x - y|$$

the *fill-distance* of  $X$  in  $\Gamma$ .

**Proposition 3.6** ([36, Theorem 2.6]). *Let  $\Gamma \subset \mathbb{R}^d$  be a bounded Lipschitz domain. There exists  $h_0 > 0$  such that, for any finite set  $X \subset \Gamma$  with  $h_{X,\Gamma} < h_0$  and any  $r \in H^{\beta}(\Gamma)$ , we have*

$$\|r\|_{L^2(\Gamma)} \lesssim_{h,r} h_{X,\Gamma}^{\beta} \|r\|_{H^{\beta}(\Gamma)} + \max_{x \in X} |r(x)|$$

□

**Proposition 3.7.** *Let  $\Gamma \subset \mathbb{R}^d$  be a bounded Lipschitz domain, and let  $\Phi$  be a reproducing kernel such that  $\mathcal{N}_{\Phi}(\Gamma) \simeq H^{\beta}(\Gamma)$ . For any  $0 \leq \alpha \leq \beta$  we have*

$$\|\text{Id} - S_X\|_{H^{\beta}(\Gamma) \rightarrow H^{\alpha}(\Gamma)} \lesssim_X h_{X,\Gamma}^{\beta-\alpha},$$

where  $S_X$  is the best-approximation in  $H^{\beta}(\Gamma)$  associated to point evaluations in  $X \subset \Gamma$ .

*Proof.* By the Gagliardo-Nirenberg interpolation inequality [21, Theorem 1], it suffices to consider the cases  $\alpha = 0$  and  $\alpha = \beta$ . For the first case, consider  $u \in H^{\beta}(\Gamma)$  and apply Proposition 3.6 to  $r := u - S_X u$ . The claim follows because  $r|_X \equiv 0$  and

$$\|r\|_{H^{\beta}(\Gamma)} \leq \|u\|_{H^{\beta}(\Gamma)} + \|S_X u\|_{H^{\beta}(\Gamma)} \leq 2\|u\|_{H^{\beta}(\Gamma)}$$

by the definition of  $S_X u$ . The second case follows directly from the previous inequality. □

We now consider the sparse approximation of functions in a native space  $\mathcal{N}_\Phi(\Gamma)$  on a product domain  $\Gamma := \prod_{j=1}^n \Gamma_j$  with a tensor product kernel  $\Phi := \Phi_1 \otimes \cdots \otimes \Phi_n: \Gamma \times \Gamma \rightarrow \mathbb{R}$ .

Since

$$\text{Id}_{\mathcal{N}_\Phi(\Gamma)} = \text{Id}_{\mathcal{N}_{\Phi_1}(\Gamma_1)} \otimes \cdots \otimes \text{Id}_{\mathcal{N}_{\Phi_n}(\Gamma_n)},$$

we may apply Smolyak's algorithm to the multilinear tensor product of operators, and we obtain an approximation of the identity operator  $\text{Id}_{\mathcal{N}_\Phi(\Gamma)}$  that employs point evaluations in a *sparse grid* [30, 22, 7].

Before we become more specific, let us recall the tensor product of operators.

**Proposition 3.8** ([13, Proposition 4.127]). *Let  $H^{(j)}$  and  $G^{(j)}$ , with  $j \in \{1, \dots, n\}$ , be Hilbert spaces and denote by  $H = \bigotimes_{j=1}^n H^{(j)}$  and  $G = \bigotimes_{j=1}^n G^{(j)}$  their Hilbert tensor products. Given operators  $\{A^{(j)}\}_{j=1}^n \in \prod_{j=1}^n \mathcal{L}(H^{(j)}, G^{(j)})$ , we define the tensor product operator on the algebraic tensor product of  $\{H^{(j)}\}_{j=1}^n$  by*

$$\left( \bigotimes_{j=1}^n A^{(j)} \right) \left( \bigotimes_{j=1}^n h^{(j)} \right) := \bigotimes_{j=1}^n A^{(j)} h^{(j)}$$

and by multilinear extension. This algebraic tensor product operator satisfies

$$\left\| \bigotimes_{j=1}^n A^{(j)} \right\|_{H \rightarrow G} = \prod_{j=1}^n \|A^{(j)}\|_{H^{(j)} \rightarrow G^{(j)}}$$

on its domain of definition and can therefore be extended to the completion  $H$ , satisfying the same bound.  $\square$

Now consider the case where the factors  $\mathcal{N}_{\Phi_j}(\Gamma_j)$  are isotropic Sobolev spaces  $H^{\beta_j}(\Gamma_j)$ ,  $\Gamma_j \subset \mathbb{R}^{d_j}$ , and we apply Smolyak's algorithm to approximate

$$v := \mathcal{M}(\text{Id}_{H^{\beta_1}(\Gamma_1)}, \dots, \text{Id}_{H^{\beta_n}(\Gamma_n)}) := \text{Id}_{H^{\beta_1}(\Gamma_1)} \otimes \cdots \otimes \text{Id}_{H^{\beta_n}(\Gamma_n)} = \text{Id}_{H_D^\beta(\Gamma)} \in \mathcal{L}(H_D^\beta(\Gamma), H_D^\alpha(\Gamma)).$$

Here, we consider  $\text{Id}_{H_D^\beta(\Gamma)}$  as taking values in  $H_D^\alpha(\Gamma)$  with  $\alpha \leq \beta$  in order to later obtain bounds in the norm of  $H_D^\alpha(\Gamma)$ . To approximate the inputs  $\text{Id}_{H^{\beta_j}(\Gamma_j)}$  we use best-approximations  $S_N^{(j)}$  associated with point evaluations in sets  $X_N^{(j)} \subset \Gamma_j$  with  $|X_N^{(j)}| = N$  and  $h_{X_N^{(j)}, \Gamma_j} \lesssim_N N^{-1/d}$ .

To be able to apply the general theory of Section 2, we need to verify the four assumptions from Section 2. Assumption 1 on the continuity of  $\mathcal{M}$  holds by Proposition 3.8 above.

Assumption 2 on the convergence of the input approximations has been established in Proposition 3.7. Finally, to satisfy Assumptions 3 and 4 we assign as work to each point evaluation a unit cost, that is

$$\text{Work}(S_N^{(j)}) := N,$$

and

$$\text{Work}(S_{N^{(1)}}^{(1)} \otimes \cdots \otimes S_{N^{(n)}}^{(n)}) := \prod_{j=1}^n N^{(j)}.$$

This is indeed the number of point evaluations required by the tensor product operator: By Proposition 3.3,  $S_{N^{(j)}}^{(j)}$  can be written as

$$\sum_{i=1}^{N^{(j)}} s_i^{(j)} \delta_{x_i^{(j)}}$$

for  $x_i^{(j)} \in X_{N^{(j)}}^{(j)}$  and some  $s_i^{(j)} \in \mathcal{N}_{\Phi_j}(\Gamma_j)$ , thus,

$$S_{N^{(1)}}^{(1)} \otimes \cdots \otimes S_{N^{(n)}}^{(n)} = \sum_{i_1=1}^{N^{(1)}} \cdots \sum_{i_n=1}^{N^{(n)}} \left( \bigotimes_{j=1}^n s_{i_j}^{(j)} \right) \delta_{(x_{i_1}^{(1)}, \dots, x_{i_n}^{(n)})}.$$

Therefore, Theorem 3.9 below follows directly from Theorem 2.1.

**Theorem 3.9. (Sparse kernel-based approximations)** Assume  $0 \leq \alpha < \beta$ . For small enough  $\epsilon$ , we can choose  $L$  such that Smolyak's algorithm with threshold  $L$  satisfies

$$\|\text{Id} - \mathcal{S}_L(\text{Id})\|_{H_D^\beta(\Gamma) \rightarrow H_D^\alpha(\Gamma)} \leq \epsilon$$

and employs

$$N_{\mathcal{S}_L(\text{Id})} \lesssim_\epsilon \epsilon^{-\rho} |\log \epsilon|^{(1+\rho)(n_0-1)} \quad (18)$$

point evaluations in  $\Gamma$ , where

$$\rho := \max_{j=1}^n d_j / (\beta_j - \alpha_j) \text{ and } n_0 := |\{j : d_j / (\beta_j - \alpha_j) = \rho\}|.$$

□

**Remark 6. (Convergence in non-Hilbert norms)** The previous theorem is an extension of Theorem 4.41 in [26], which provides  $L^\infty$  bounds for interpolation in an  $n$ -fold tensor product of a univariate Sobolev space.

To derive bounds on the error in non-Hilbert norms, such as  $L^\infty$ , observe that the proof of Proposition 3.7 goes through for non-Hilbert Sobolev spaces whose parameters satisfy certain conditions determined by the Gagliardo-Nirenberg inequality. It remains to be checked whether the desired norm is uniform with the native space norm in the sense introduced in Section 2. For bounds in the  $L^\infty$ -norm, one can simply use pointwise estimates and the fact that  $\mathbb{R} = \mathbb{R} \otimes \cdots \otimes \mathbb{R}$  is a Hilbert tensor product. In this case, the result in Equation (18) holds true with

$$\rho := \max_{j=1}^n d_j / (\beta_j - d_j/2) \text{ and } n_0 := |\arg \max_{j=1}^n \{d_j / (\beta_j - d_j/2)\}|.$$

**Remark 7. (Exponential convergence)** In [6, 4], Smolyak's algorithm is applied to approximation with Gaussian kernels (which have exponential univariate convergence rates). Theorem 4.44 in [26] claims that using  $h_l := h_{X_l^{(j)}, \Gamma_j} \leq \exp(-l)$  yields exponential convergence in terms of the required samples,  $\exp(-cN)$ , when Smolyak's algorithm is applied to the  $n$ -fold tensor product of univariate Gaussian kernel native spaces. However, the proof is based on the claim that the univariate interpolants satisfy

$$\|\text{Id} - S_l^{(j)}\| \leq c_\phi h_l^k \quad \forall l, k \in \mathbb{N} \quad (19)$$

for constants  $c_\phi, C, c$  independent of  $k$  and  $l$ , such that

$$c_\phi h_l^k \leq C \exp(-ch_l^{-1}) \quad \forall l, k \in \mathbb{N}, \quad (20)$$

which seems to be incorrect (consider  $h_l < 1$  and  $k \rightarrow \infty$ ). Indeed the Smolyak algorithm with  $N_l^{(j)} \approx \exp(t_j l)$  is tailored to the situation of algebraically converging approximations and algebraically diverging work. To group contributions with equal work-to-error ratio as in Equation (6), if the error converges exponentially and the work grows algebraically, one should use arithmetic subsequences  $N_l^{(j)} \approx ml$ . This yields only sub-exponential convergence,  $\exp(-cN^{1/n})$ , as does approximation with Gaussian kernels and quasi-uniform point sets. However, it can be shown that the factor  $c = c(n)$  behaves better for large values of  $n$  [10].

## 4 Applications to parametric and random PDEs

We apply Smolyak's algorithm to parametric partial differential equations of the form

$$P_y(u) = f_y \quad (21)$$

where both the partial differential operator  $P_y$  and the right-hand side  $f_y$  depend on a parameter  $y \in \Gamma \subset \mathbb{R}^d$ .

Assuming that there is a unique solution  $u_y := P_y^{-1}(f_y)$  for each  $y \in \Gamma$ , our goal is to approximate the dependence of a scalar, possibly nonlinear, quantity of interest  $Q(u_y)$  on the parameter  $y$ .

### 4.1 Approximation of expectations

In this subsection, we assume that the parameter space  $\Gamma \subset \mathbb{R}^d$  is equipped with a probability distribution  $\pi$ , and our goal is to approximate expected values of quantities of interest. We show how multilevel and multi-index methods can be regarded as applications of Smolyak's algorithm to generalized multilinear approximation problems. While the resulting methods are not new, we obtain streamlined proofs and see that linearity of the underlying PDE is not required to obtain multilinear approximation problems.

Our goal is to compute the expectation  $E[Q(P_y^{-1}(f_y))] = \int Q(P_y^{-1}(f_y))d\pi(y)$ . If  $Q$  is sufficiently smooth and  $P_y$  and  $f_y$  depend nicely on  $y$ , then

$$\begin{aligned} q: \Gamma &\rightarrow \mathbb{R} \\ y &\mapsto q(y) := Q(P_y^{-1}(f_y)) \end{aligned}$$

does as well, and is an element of some space  $H$  of regular functions from  $\Gamma$  to  $\mathbb{R}$ .

In practice, we cannot compute  $P_y^{-1}$  exactly but instead we have to rely on discretizations  $P_{y,N^{(2)}}^{-1}$ , corresponding to a numerical solver with  $N^{(2)}$  mesh points and coefficients determined by  $y$ . This yields approximations  $q_{N^{(2)}} \in H$  of  $q$ , defined by

$$q_{N^{(2)}}(y) := Q(P_{y,N^{(2)}}^{-1}f_y).$$

Furthermore, we cannot compute approximations to the solution for all values of  $y$ , but only for  $N^{(1)}$  samples and then need to rely on quadrature rules  $\mathcal{I}_{N^{(1)}}: H \rightarrow \mathbb{R}$  based on these samples. A straightforward approximation of  $E[q]$  is then

$$E[q] \approx \mathcal{I}_{N^{(1)}}q_{N^{(2)}} \quad (22)$$

for large  $N^{(1)}$  and  $N^{(2)}$ , corresponding to many samples of a fine discretization of the PDE.

To obtain approximations that achieve the same error with less work, we observe that

$$\begin{aligned} \mathcal{B}: \mathcal{L}(H, \mathbb{R}) \times H &\rightarrow \mathbb{R} \\ (\lambda, h) &\mapsto \lambda h \end{aligned}$$

is a continuous bilinear form and our goal is to approximate

$$v := E[q] = \mathcal{B}(E, q) \in \mathbb{R}$$

using the approximations  $\mathcal{I}_N$  of  $E$  and  $q_N$  of  $q$ . This is exactly the setting of Section 2, with Assumption 1 on the continuity of the bilinear form corresponding to the definition of operator norms. To satisfy Assumptions 2 to 4 on error and work, we require

$$\|E - \mathcal{I}_N\|_{H \rightarrow \mathbb{R}} \lesssim_N N^{-\beta},$$

$$\|q - q_N\|_H \lesssim_N N^{-\kappa},$$

and that an approximation of the solution of the PDE with a fixed parameter  $y \in \Gamma$  and  $N$  mesh points requires the work  $N^\gamma$ . Furthermore, we associate with  $\mathcal{I}_{N^{(1)}}$  the work  $N^{(1)}$ , with  $q_{N^{(2)}}$  the work  $(N^{(2)})^\gamma$ , and with  $\mathcal{I}_{N^{(1)}}q_{N^{(2)}}$  the work  $N^{(1)}(N^{(2)})^\gamma$  required for  $N^{(1)}$  calls of the PDE solver with  $N^{(2)}$  mesh points. Theorem 2.1 now shows that for small enough  $\epsilon$ , we may choose  $L$  such that Smolyak's algorithm

$$\mathcal{S}_L(v) := \sum_{|l|_1 \leq L} \Delta_{l_1}^{(1)} \Delta_{l_2}^{(2)} = \sum_{l=1}^{L-1} \mathcal{I}_l \Delta_{L-l}^{(2)} \quad (23)$$

achieves an error of size  $\epsilon > 0$  with work

$$\epsilon^{-\rho} |\log \epsilon|^{(1+\rho)(n_0-1)}, \quad (24)$$

where

$$\rho := \max\{\gamma/\kappa, 1/\beta\}, n_0 := |\arg \max\{\gamma/\kappa, 1/\beta\}|.$$

Using the straightforward approximation from Equation (22) instead would require the work  $\epsilon^{-\gamma/\kappa-1/\beta}$ .

Equation (23) is the celebrated *multilevel formula* [9] and Equation (24) agrees with the work analysis in [32]. Strictly speaking, [9, 32, 20] allow for weak and strong convergence rates. If these differ and if  $\gamma/\kappa > 1/\beta$ , then the result can be slightly improved by a more elaborate analysis. Furthermore, the multilevel formula of [9] was formulated for Monte Carlo sampling. We show in Section 4.3 how such random sampling and corresponding probabilistic results can be obtained in the framework of multilinear approximation problems. First, we expand on the case of deterministic quadrature rules on domains in  $\mathbb{R}^d$ . In the case of separable probability densities, we can interpret the multidimensional integral operator as a tensor product of lower-dimensional integral operators and this multilinear structure allows for further sparsification of the approximation. More specifically, we consider the case where the integration domain is a cartesian product,  $\Gamma = \prod_{j=1}^n \Gamma^{(j)}$  with  $\Gamma^{(j)} \subset \mathbb{R}^{d_j}$ , and where

$$H = H_D^\beta(\Gamma) = \bigotimes_{j=1}^n H^{\beta_j}(\Gamma^{(j)}),$$

which is a tensor product Sobolev space as in Section 3. Furthermore, we assume that the distribution  $\pi$  of  $y$  is separable,  $\pi = \prod_{j=1}^n \pi^{(j)}$ . Since the operators  $\bigotimes_{j=1}^n \int_{\Gamma^{(j)}} d\pi^{(j)}$  and  $\int_\Gamma d\pi$  agree on elementary tensors by Fubini's theorem, they are equal, and we may consider the multilinear approximation problem

$$E[q] = \left( \bigotimes_{j=1}^n \int_{\Gamma^{(j)}} d\pi^{(j)} \right) q =: \mathcal{M} \left( \int_{\Gamma^{(1)}} d\pi^{(1)}, \dots, \int_{\Gamma^{(n)}} d\pi^{(n)}, q \right).$$

This time we form Smolyak's algorithm based on the  $(n+1)$ -linear map  $\mathcal{M}$  and on quadrature rules  $\mathcal{I}_N^{(j)}: H^{\beta_j}(\Gamma^{(j)}) \rightarrow \mathbb{R}$ . We maintain the assumption that

$$\|q - q_N\|_{H_D^\beta(\Gamma)} \lesssim_N N^{-\kappa}. \quad (25)$$

and further assume that

$$\left\| \int_{\Gamma^{(j)}} d\pi^{(j)} - \mathcal{I}_N^{(j)} \right\|_{H^{\beta_j}(\Gamma^{(j)}) \rightarrow \mathbb{R}} \lesssim_N N^{-\beta_j/d_j} \quad (26)$$

for  $j \in \{1, \dots, n\}$ . For example, if  $\pi^{(j)}$  has a bounded density with respect to the Lebesgue measure, we can use for  $\mathcal{I}_N^{(j)}$  the integral over the kernel-based best-approximation associated with point evaluations in  $Y_N^{(j)} \subset \Gamma^{(j)}$  with  $h_{Y_N^{(j)}, \Gamma^{(j)}} \lesssim_N N^{-1/d_j}$ . In any case, we assume that the resulting quadrature points and weights are calculated beforehand. Smolyak's algorithm in this setting yields the Multi-index Stochastic Collocation method, which was introduced in [15, 16]. By presenting this method in the general framework of Smolyak's algorithm, we obtain a succinct proof of its convergence. Indeed, the convergence rate in Theorem 4.1 below agrees with that in [15, Theorem 1].

**Theorem 4.1.** *Let  $q_N$ ,  $\mathcal{I}_N$ , and  $\mathcal{M}$  be as above. In particular, assume that the estimates in Equations (25) and (26) hold and that each call of the PDE solver to obtain a sample  $q_N(y)$ ,  $y \in \Gamma$ , requires the computational work  $\tau \lesssim_N N^\gamma$ . For small enough  $\epsilon > 0$ , we can choose  $L$  such that Smolyak's algorithm  $\mathcal{S}_L := \mathcal{S}_L(E[q])$  with work parameters  $(1, \dots, 1, \gamma)$  and convergence parameters  $(\beta_1/d_1, \dots, \beta_n/d_n, \kappa)$  achieves*

$$|E[q] - \mathcal{S}_L| \leq \epsilon$$

with the computational work bounded by

$$\text{Work}(\mathcal{S}_L) \lesssim_\epsilon \epsilon^{-\rho} |\log \epsilon|^{(1+\rho)(n_0-1)}, \quad (27)$$

where

$$\rho := \max\{d_1/\beta_1, \dots, d_n/\beta_n, \gamma/\kappa\}$$

and

$$n_0 = |\arg \max\{d_1/\beta_1, \dots, d_n/\beta_n, \gamma/\kappa\}|.$$

*Proof.* We check the assumptions of Section 2. For this purpose, we view  $\mathcal{M}$  as a multilinear map

$$\mathcal{M}: \left( \prod_{j=1}^n \mathcal{L}(H^{\beta_j}(\Gamma_j), \mathbb{R}) \right) \times H_D^\beta(\Gamma) \rightarrow \mathbb{R}.$$

Assumption 1 on the continuity of  $\mathcal{M}$  follows from Proposition 3.8 together with the definition of the operator norm: For arbitrary elements  $\lambda^{(j)} \in \mathcal{L}(H^{\beta_j}(\Gamma_j), \mathbb{R})$  and  $h \in H_D^\beta(\Gamma)$  we have

$$\begin{aligned} |\mathcal{M}(\lambda^{(1)}, \dots, \lambda^{(n)}, h)| &\leq \left\| \bigotimes_{j=1}^n \lambda^{(j)} \right\|_{H_D^\beta(\Gamma) \rightarrow \mathbb{R}} \|h\|_{H_D^\beta(\Gamma)} \\ &\leq \prod_{j=1}^n \|\lambda^{(j)}\|_{H^{\beta_j}(\Gamma_j) \rightarrow \mathbb{R}} \|h\|_{H_D^\beta(\Gamma)}. \end{aligned}$$

Assumption 2 follows from Equations (25) and (26). Finally, we assign as work to  $\mathcal{I}_N^{(j)}$  the number of required point evaluations  $N$ , to  $q_N$  the computational work  $N^\gamma$ , and to the evaluation of

$$\mathcal{M}(\mathcal{I}_{N^{(1)}}^{(1)}, \dots, \mathcal{I}_{N^{(n)}}^{(n)}, q_{N^{(n+1)}})$$

the product

$$\left( \prod_{j=1}^n N^{(j)} \right) (N^{(n+1)})^\gamma,$$

which is the computational work required by  $\prod_{j=1}^n N^{(j)}$  calls of the PDE solver with  $N^{(n+1)}$  mesh points. Therefore, all Assumptions of Section 2 are satisfied and the claim follows from Theorem 2.1.  $\square$

## 4.2 Response surface approximation

Our general formulation of Smolyak's algorithm allows us to extend the multilevel and multi-index methods of the previous subsection to the approximation of the full response surface  $q: \Gamma \rightarrow \mathbb{R}$  without much effort, provided we have an interpolation method which converges to the identity with an algebraic rate. We give below a result using kernel-based approximations (see Section 3).

As before, we assume that  $q \in H_D^\beta(\Gamma)$ , where  $\Gamma = \prod_{j=1}^n \Gamma^{(j)}$  and  $\Gamma^{(j)} \subset \mathbb{R}^{d_j}$  are Lipschitz domains and  $\beta = (\beta_1, \dots, \beta_n) > (d_1/2, \dots, d_n/2)$ . To apply Smolyak's algorithm we observe that

$$q = \text{Id } q = \left( \bigotimes_{j=1}^n \text{Id}^{(j)} \right) q =: \mathcal{M}(\text{Id}^{(1)}, \dots, \text{Id}^{(n)}, q),$$

where  $\text{Id}^{(j)}$ ,  $j \in \{1, \dots, n\}$ , is the identity on  $H^{\beta_j}(\Gamma_j)$ , which we approximate by the best-approximations  $S_N^{(j)}$  from Section 3 based on evaluations in  $Y_N^{(j)} \subset \Gamma^{(j)} \subset \mathbb{R}^{d_j}$  such that  $h_{Y_N^{(j)}, \Gamma^{(j)}} \lesssim_N N^{-1/d_j}$ .

**Theorem 4.2.** *Suppose that we have convergence  $q_N \rightarrow q$  as specified in Equation (25), and that each call of the PDE solver to obtain a sample  $q_N(y)$ ,  $y \in \Gamma$ , requires the computational work  $\tau \lesssim_N N^\gamma$ . Let  $0 \leq \alpha < \beta$ . For small enough  $\epsilon > 0$  we can choose  $L$  such that Smolyak's algorithm  $\mathcal{S}_L := \mathcal{S}_L(q)$  with work parameters  $(1, \dots, 1, \gamma)$  and convergence parameters  $((\beta_1 - \alpha_1)/d_1, \dots, (\beta_n - \alpha_n)/d_n, \kappa)$  satisfies*

$$\|q - \mathcal{S}_L\|_{H_D^\alpha(\Gamma)} \leq \epsilon$$

and such that the computational work spent on calls of the PDE solver is bounded by

$$W(\mathcal{S}_L) \lesssim_{\epsilon} \epsilon^{-\rho} |\log \epsilon|^{(1+\rho)(n_0-1)}, \quad (28)$$

where

$$\rho := \max\{d_1/(\beta_1 - \alpha_1), \dots, d_n/(\beta_n - \alpha_n), \gamma/\kappa\}$$

and

$$n_0 = |\arg \max\{d_1/(\beta_1 - \alpha_1), \dots, d_n/(\beta_n - \alpha_n), \gamma/\kappa\}|.$$

*Proof.* As before, Assumption 1 of Section 2 holds since the multilinear map

$$\begin{aligned} \mathcal{M}: \left( \prod_{j=1}^n \mathcal{L}(H^{\beta_j}(\Gamma_j), H^{\alpha_j}(\Gamma_j)) \right) \times H_D^{\beta}(\Gamma) &\rightarrow H_D^{\alpha}(\Gamma) \\ \left( (A^{(j)})_{j=1}^n, h \right) &\mapsto \left( \bigotimes_{j=1}^n A^{(j)} \right) h \end{aligned}$$

is continuous by Proposition 3.8.

Assumption 2 of Section 2 holds for  $q_N$  by assumption and for  $S_N^{(j)}$ ,  $j \in \{1, \dots, n\}$ , by Proposition 3.7, which states that

$$\|\text{Id}^{(j)} - S_N^{(j)}\|_{H^{\beta_j}(\Gamma^{(j)}) \rightarrow H^{\alpha_j}(\Gamma^{(j)})} \lesssim_N N^{-(\beta_j - \alpha_j)/d_j}.$$

Finally, we associate as work to  $S_N^{(j)}$  the number of required point evaluations  $N$ , to  $q_N$  the work  $N^{\gamma}$ , and to the evaluation of

$$\mathcal{M}(S_{N^{(1)}}^{(1)}, \dots, S_{N^{(n)}}^{(n)}, q_{N^{(n+1)}})$$

the product

$$\left( \prod_{j=1}^n N^{(j)} \right) (N^{(n+1)})^{\gamma},$$

which is the computational work required for  $\prod_{j=1}^n N^{(j)}$  samples of  $q_{N^{(n+1)}}$ . Therefore all Assumptions of Section 2 are satisfied and the claim follows from Theorem 2.1.  $\square$

**Remark 8. (Total work)** In practice, additionally to calls of the PDE solver, we need to determine the elements  $s_{i,N}^{(j)} \in H^{\beta_j}(\Gamma_j)$  in

$$S_N^{(j)} f = \sum_{i=1}^N s_{i,N}^{(j)} f(y_{i,N}^{(j)}), \quad (29)$$

using Proposition 3.3. Denote the computational work required for this computation by  $\tau_S$  and denote by  $\tau_P$  the computational work required for all calls of the PDE solver, for which we use the estimate

$$\tau_P \lesssim_L \exp(Lg) L^{n_0-1} \quad (30)$$

from Equation (9), where  $g = \max \mathbf{g}$  and  $n_0 = |\arg \max \mathbf{g}|$  with

$$\mathbf{g} = (1/(1 + (\beta_1 - \alpha_1)/d_1), \dots, 1/(1 + (\beta_n - \alpha_n)/d_n), \gamma/(\gamma + \kappa)).$$

If we can solve the linear systems of Proposition 3.3 of size  $N$  in time  $N^{\lambda}$ , then (recall the definition  $N_l^{(j)} := \exp(l/(1 + (\beta_j - \alpha_j)/d_j))$  from Section 2)

$$\tau_S = \sum_{j=1}^n \sum_{l=1}^L \left( N_l^{(j)} \right)^{\lambda} \lesssim_L \sum_{l=1}^L \exp(l\tilde{g}) \lesssim_L \exp(L\tilde{g}), \quad (31)$$



where  $\tilde{g} := \lambda \max_{j=1}^n \{1/(1 + (\beta_j - \alpha_j)/d_j)\}$ . Comparison of Equations (30) and (31) shows that  $\tau_S$  is negligible if

$$\tilde{g} \leq \gamma/(\gamma + \kappa).$$

In all other cases, we need to assume that the elements  $s_{i, N_i^{(j)}}^{(j)}$  were computed off-line.

### 4.3 Optimization under uncertainty

We now consider the case where the parameter  $y = (z, m)$  in Equation (21) can be split into a deterministic component  $z$  and a random component  $m$ . Taking expectation over the random component and optimizing over the deterministic one then gives rise to a problem of optimization under uncertainty [24, 28, 29, 1].

We assume that  $m$  is a random element over a probability space  $(\Omega, \mathcal{A}, P)$  with values in a possibly infinite-dimensional Banach space.

Our goal is to solve the minimization problem

$$\min_{z \in \Gamma} v(z) + \psi(z),$$

where

$$v(z) := E[Q(u_{(z,m)})]$$

is the expected value with respect to  $P$ , and  $\psi$  depends only on the deterministic parameter  $z$ , acting as a penalty term for large  $z$  for example. Difficulties in this minimization problem arise for similar reasons as before:

- Given  $z$  and  $m$ , we can only compute approximations  $u_{(z,m),N} := P_{(z,m),N}^{-1} f_{(z,m)}$  to the solution of the PDE.
- Since  $m$  is a random element, we need to rely on sampling strategies to approximate the expected value. In this section we show how Monte Carlo sampling can be included in the framework of general multilinear problems; however, deterministic sampling strategies as in Section 4.1 may be applied alternatively.
- As a consequence we can only compute approximations of  $v(z)$ , and we can only do so for few values of  $z$ .

To address these issues, we propose a method for the computation of surrogate models that converge to  $Q$  with high probability. These surrogate models are given in terms of their coefficients with respect to a basis of kernel functions. As such they can be evaluated with relatively low computational effort and minimized by standard techniques.

As in previous sections, we assume that  $\Gamma = \prod_{j=1}^n \Gamma^{(j)}$  for Lipschitz domains  $\Gamma^{(j)} \subset \mathbb{R}^{d_j}$ ,  $v \in H_D^\beta(\Gamma)$  for some partition  $D$  of  $\{1, \dots, d\}$ , and  $\beta = (\beta_1, \dots, \beta_n) > (d_1/2, \dots, d_n/2)$  to assure that pointwise evaluations are possible. Furthermore, we assume that for  $P$ -almost all  $\omega \in \Omega$  we have

$$\tilde{v}(\omega) := (z \mapsto Q(u_{(z,m(\omega))})) \in H_D^\beta(\Gamma)$$

and  $\tilde{v}$  is an element of the Bochner space  $L^2(\Omega; H_D^\beta(\Gamma))$ . To obtain a multilinear approximation problem, we consider the problem of approximating the constant  $H_D^\beta(\Gamma)$ -valued random variable

$$v = \mathcal{M}(\text{Id}^{(1)}, \dots, \text{Id}^{(n)}, E, \tilde{v}) := \left( \text{Id}^{(1)} \otimes \dots \otimes \text{Id}^{(n)} \right) E[\tilde{v}] \in L^2(\Omega^\mathbb{N}; H_D^\beta(\Gamma)),$$

where

- $(\Omega^\mathbb{N}, \mathcal{A}^\mathbb{N}, P^\mathbb{N})$  is the  $\mathbb{N}$ -fold product probability space with product measure, representing a sequence of independent and identically distributed draws of  $m$
- we regard expectation as an operator

$$E: L^2(\Omega; H_D^\beta(\Gamma)) \rightarrow L^2(\Omega^\mathbb{N}; H_D^\beta(\Gamma)),$$

which maps elements of the Bochner space  $L^2(\Omega; H_D^\beta(\Gamma))$  to their expected value, regarded as deterministic element of  $L^2(\Omega^\mathbb{N}; H_D^\beta(\Gamma))$

- $\text{Id}^{(j)}$  is the identity on  $H^{\beta_j}(\Gamma_j)$  for  $j \in \{1, \dots, n\}$ .

To apply Smolyak's algorithm, we use the following approximations

- To approximate  $\tilde{v}$ , we use the random variable

$$\tilde{v}_N(\omega) := (z \mapsto Q(u_{(z, m(\omega)), N}))$$

- To approximate the expectation operator  $E$ , we use the empirical mean operators

$$\begin{aligned} \Xi_N: L^2(\Omega; H_D^\beta(\Gamma)) &\rightarrow L^2(\Omega^\mathbb{N}; H_D^\beta(\Gamma)), \\ (\Xi_N X)(\omega) &:= \frac{1}{N} \sum_{i=1}^N X(\omega_i) \quad \forall \omega \in \Omega^\mathbb{N} \end{aligned}$$

- To approximate the identities  $\text{Id}^{(j)}$ , we use the best-approximations  $S_N^{(j)}$  from Section 3 based on sets  $Z_N^{(j)} \subset \Gamma^{(j)} \subset \mathbb{R}^{d_j}$  with fill-distances

$$h_{Z_N^{(j)}, \Gamma^{(j)}} \lesssim_N N^{-1/d_j}.$$

Smolyak's algorithm applied to this setting yields random elements in  $H_D^\beta(\Gamma)$  that converge to the deterministic function  $v \in H_D^\beta(\Gamma)$  in the probabilistic mean squared error (MSE) as  $L \rightarrow \infty$ .

Before we prove this convergence, we describe Smolyak's algorithm from a computational perspective. If we denote the members of  $Z_N^{(j)}$  by  $(z_{i,N}^{(j)})_{i=1}^N$ , then by Proposition 3.3 each  $S_N^{(j)}$  can be written as

$$S_N^{(j)} f = \sum_{i=1}^N s_{i,N}^{(j)} f(z_{i,N}^{(j)}), \quad (32)$$

with  $s_{i,N}^{(j)} \in H^{\beta_j}(\Gamma^{(j)})$ . The value  $\mathcal{M}(S_{N^{(1)}}^{(1)}, \dots, S_{N^{(n)}}^{(n)}, \Xi_{N^{(n+1)}}, \tilde{v}_{N^{(n+2)}})$ , which is formally defined as an element of  $L^2(\Omega^\mathbb{N}; H_D^\beta(\Gamma))$ , is therefore given by

$$\sum_{i \in \mathcal{J}} s_i \frac{1}{N^{(n+1)}} \sum_{k=1}^{N^{(n+1)}} Q(u_{(z_i, m(\omega_k)), N^{(n+2)}}) \quad (33)$$

where

$$\mathcal{J} := \{i \in \mathbb{N}^n : 1 \leq i_j \leq N^{(j)}\},$$

$$s_i := \bigotimes_{j=1}^n s_{i_j, N^{(j)}}^{(j)},$$

and

$$z_i := (z_{i_1, N^{(1)}}^{(1)}, \dots, z_{i_n, N^{(n)}}^{(n)}).$$

This means that we draw independent samples  $(m(\omega_k))_{k=1}^{N^{(n+1)}}$  of  $m$  and then form a kernel interpolant based on the averaged values  $(\frac{1}{N^{(n+1)}} \sum_{k=1}^{N^{(n+1)}} Q(u_{(z_i, m(\omega_k)), N^{(n+2)}}))_{i \in \mathcal{J}}$ . From the combination rule in Equation (14), we see that Smolyak's algorithm is a linear combination of approximations as in Equation (33).

**Theorem 4.3.** *Let  $0 \leq \alpha \leq \beta$ . Assume that*

$$\sup_m \|Q(u_{(\cdot, m)}) - Q(u_{(\cdot, m), N})\|_{H_D^\beta(\Gamma)} \lesssim_N N^{-\kappa}$$

*and assume that each call of the PDE solver to obtain  $u_{(z, m), N}$  given  $z$  and  $m$  requires the computational work  $\tau \lesssim_N N^\gamma$ . For small enough  $\epsilon > 0$  we can choose  $L$  such that the Smolyak*

algorithm  $\mathcal{S}_L := \mathcal{S}_L(v)$  with work parameters  $(1, \dots, 1, 1, \gamma)$  and convergence parameters  $((\beta_1 - \alpha_1)/d_1, \dots, (\beta_n - \alpha_n)/d_n, 1/2, \kappa)$  satisfies

$$\mathbb{E}[\|v - \mathcal{S}_L\|_{H_D^\alpha(\Gamma)}^2] \leq \epsilon^2 \quad (34)$$

and such that the computational work required for all calls of the PDE solver is bounded by

$$\text{Work}(\mathcal{S}_L) \lesssim_\epsilon \epsilon^{-\rho} |\log \epsilon|^{(1+\rho)(n_0-1)}, \quad (35)$$

where

$$\rho := \max\{d_1/(\beta_1 - \alpha_1), \dots, d_n/(\beta_n - \alpha_n), 2, \gamma/\kappa\}$$

and

$$n_0 = \lceil \arg \max\{d_1/(\beta_1 - \alpha_1), \dots, d_n/(\beta_n - \alpha_n), 2, \gamma/\kappa\} \rceil.$$

By Chebyshev's inequality, for example, Equation (34) implies

$$P(\|v - \mathcal{S}_L\|_{H_D^\alpha(\Gamma)} \geq \delta) \leq \frac{\epsilon^2}{\delta^2}.$$

*Proof.* We check the assumptions of Section 2 for the multilinear map

$$\begin{aligned} \mathcal{M}: \left( \prod_{j=1}^n \mathcal{L}(H^{\beta_j}(\Gamma_j), H^{\alpha_j}(\Gamma_j)) \right) \times \mathcal{L}\left(L^2(\Omega; H_D^\beta(\Gamma)), L^2(\Omega^\mathbb{N}; H_D^\beta(\Gamma))\right) \times L^2(\Omega, H_D^\beta(\Gamma)) &\rightarrow L^2(\Omega^\mathbb{N}; H_D^\alpha(\Gamma)) \\ \left( (A^{(j)})_{j=1}^n, B, C \right) &\mapsto \left( \bigotimes_{j=1}^n A^{(j)} \right) B[C] \end{aligned}$$

Assumption 1 on the continuity of  $\mathcal{M}$  follows from Proposition 3.8 together with the definition of operator norms:

$$\begin{aligned} \left\| \left( \bigotimes_{j=1}^n A^{(j)} \right) B[C] \right\|_{L^2(\Omega^\mathbb{N}; H_D^\alpha(\Gamma))} &\leq \left\| \bigotimes_{j=1}^n A^{(j)} \right\|_{H_D^\beta(\Gamma) \rightarrow H_D^\alpha(\Gamma)} \|B[C]\|_{L^2(\Omega^\mathbb{N}; H_D^\beta(\Gamma))} \\ &\leq \prod_{j=1}^n \|A^{(j)}\|_{H^{\beta_j}(\Gamma_j) \rightarrow H^{\alpha_j}(\Gamma_j)} \|B\|_{L^2(\Omega; H_D^\beta(\Gamma)) \rightarrow L^2(\Omega^\mathbb{N}; H_D^\beta(\Gamma))} \|C\|_{L^2(\Omega; H_D^\beta(\Gamma))}. \end{aligned}$$

Next, we check the convergence rates of the input approximations  $S_N^{(j)} \rightarrow \text{Id}^{(j)}$ ,  $\Xi_N \rightarrow E$ , and  $\tilde{v}_N \rightarrow \tilde{v}$ .

- By Proposition 3.7, we have

$$\|\text{Id}^{(j)} - S_N^{(j)}\|_{H^{\beta_j}(\Gamma^{(j)}) \rightarrow H^{\alpha_j}(\Gamma^{(j)})} \lesssim_N N^{-(\beta_j - \alpha_j)/d_j}.$$

- By standard Monte Carlo theory, we have

$$\|E - \Xi_N\|_{L^2(\Omega; H_D^\beta(\Gamma)) \rightarrow L^2(\Omega^\mathbb{N}; H_D^\beta(\Gamma))} \lesssim_N N^{-1/2}.$$

- We have

$$\begin{aligned} \|\tilde{v} - \tilde{v}_N\|_{L^2(\Omega; H_D^\beta(\Gamma))} &\leq \sup_m \|Q(u_{(\cdot, m)}) - Q(u_{(\cdot, m), N})\|_{H_D^\beta(\Gamma)} \\ &\lesssim_N N^{-\kappa} \end{aligned}$$

by assumption.

We associate as work with the operators  $S_N^{(j)}$ ,  $j \in \{1, \dots, n\}$ , and  $\Xi_N$  the number of required evaluations  $N$ , with  $\tilde{v}_N$  the computational work  $N^\gamma$  required per sample, and, to satisfy Assumption 4 of Section 2, with

$$\mathcal{M}(S_{N^{(1)}}^{(1)}, \dots, S_{N^{(n)}}^{(n)}, \Xi_{N^{(n+1)}}, \tilde{v}_{N^{(n+2)}})$$

the product

$$\left(\prod_{j=1}^{n+1} N^{(j)}\right)(N^{(n+2)})^\gamma,$$

which is the computational work required for the calls of the PDE solver (cf. Equation (33)).  $\square$

**Remark 9. (Total work)** By the same arguments as in the remark after Theorem 4.2, the work for the computation of the elements  $s_{i,N}^{(j)}$  in Equation (32) is negligible when

$$\lambda \min_{j=1}^n \{1/(1 + (\beta_j - \alpha_j)/d_j)\} \leq \max\{2/3, \gamma/(\gamma + \kappa)\},$$

where  $N^\lambda$  is the computational work required to solve linear systems of size  $N$  in Proposition 3.3.

**Remark 10. (Convergence in  $L^\infty$ )** Analogously to the remark after Theorem 3.9, the result also holds if we measure the error in  $L^\infty(\Gamma)$ , if we change the convergence parameters to

$$((\beta_1 - d_1/2)/d_1, \dots, (\beta_n - d_n/2)/d_n, 1/2, \kappa)$$

and adapt  $\rho$  and  $n_0$  accordingly.

**Remark 11.** The recent work [3] describes a similar algorithm employing a multilevel approach to directly find minima without reconstruction of the complete response surface using the Robbins-Monro algorithm [23].

## 5 Numerical Experiments

To support our theoretical analysis, we performed numerical experiments on two linear elliptic PDEs using MATLAB on a computer with two Intel Xeon X5650 (2.66Ghz) processors.

### 5.1 Response surface approximation

We consider diffusion through a material with a number  $n$  of uncertain bumps in the diffusion coefficient, described by the partial differential equation

$$\begin{aligned} -\nabla \cdot (a_y \nabla u_y) &= 1 && \text{in } (0, 1)^2 \\ u_y &= 0 && \text{on } \partial(0, 1)^2, \end{aligned} \tag{36}$$

where the parameter  $y = (c_1, \dots, c_n) \in \Gamma^{(1)} \times \dots \times \Gamma^{(n)} \subset ([0, 1]^2)^n$  describes the centers of the bumps. These affect the diffusion coefficient additively through

$$a_y(x) = 2 + \sum_{j=1}^n \phi(x - c_j) \tag{37}$$

where  $\phi \in C_c^2(\mathbb{R}^2, \mathbb{R}_{\geq})$  is defined by  $\phi(x) := \phi_0(|x|/R)$  with  $\phi_0(r) := \int_0^{(1-r)^+} s^2(1-s)^2 ds$  and  $R = 0.25$  for  $n = 1$ ,  $R = 0.125$  otherwise. We are interested in the dependence of the spatial average

$$q(y) := Q(u_y) := \int_{(0,1)^2} u_y(x) dx \tag{38}$$

on the locations of the bumps.

For our numerical experiments, we partitioned the variables according to the bumps they describe. This means that we used kernel-based approximations  $S_N^{(j)}: H^2(\Gamma^{(j)}) \rightarrow L^2(\Gamma^{(j)})$ ,  $j \in \{1, \dots, n\}$  based on evaluations in sets  $Y_N^{(j)} \subset \Gamma^{(j)} \subset [0, 1]^2$  with  $|Y_N^{(j)}| = N$  and  $h_{Y_N^{(j)}, \Gamma^{(j)}} \lesssim_N N^{-1/2}$ . The domains  $\Gamma^{(j)} \subset [0, 1]^2$  were chosen such that the supports of  $\phi(x - c_j)$ ,  $c_j \in \Gamma^{(j)}$  did not overlap, see Figure 1.

Furthermore, we approximated  $u_y$  using the finite element method with continuous piecewise linear elements on a quasi-uniform mesh with maximal element size  $h_{\max}$  and  $M \approx h_{\max}^{-2}$  mesh points. Consequently, instead of sampling  $q$ , we relied on the approximations  $q_{h_{\max}}(y) := Q(u_{y, h_{\max}})$ .

Differentiation of Equation (36) with respect to  $y$  and subsequent calculations similar to but simpler than those in [19] show that

$$\|\partial_{\alpha} q - \partial_{\alpha} q_{h_{\max}}\|_{L^2(\Gamma)} \lesssim_{h_{\max}} h_{\max}^2 \quad (39)$$

for all  $\alpha$  such that  $\alpha_{2j-1} + \alpha_{2j} \leq 2$ ,  $j \in \{1, \dots, n\}$  (observe that under this condition on  $\alpha$  the derivative  $\partial_{\alpha} a_y$  with respect to  $y$  exists). Therefore, we have

$$\|q - q_{h_{\max}}\|_{H_D^2(\Gamma)} \lesssim_{h_{\max}} h_{\max}^2 \approx M^{-1}, \quad (40)$$

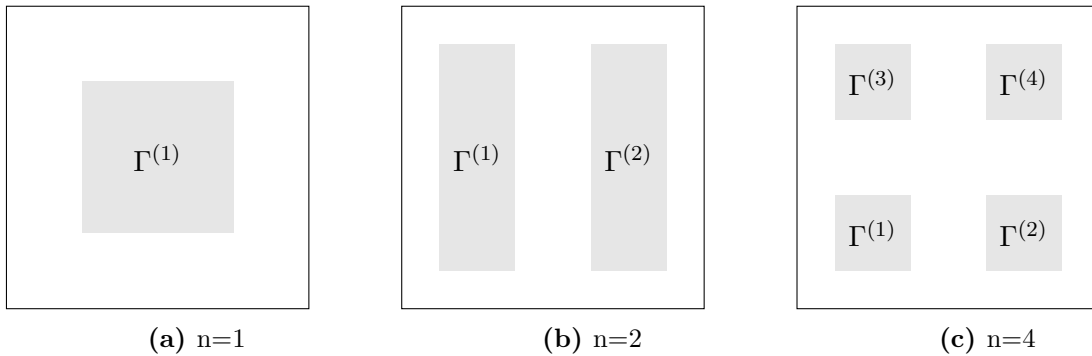
where  $H_D^2(\Gamma) = \bigotimes_{j=1}^n H^2(\Gamma^{(j)})$ .

Finally, we verified experimentally that samples of  $q_{h_{\max}}$  required approximately the runtime  $h_{\max}^{-3} = M^{3/2}$ . Consequentially, we applied Smolyak's algorithm from Section 4.2 with work parameters  $(1, \dots, 1, 3/2)$  and convergence parameters  $(2/2, \dots, 2/2, 1) = (1, \dots, 1, 1)$ . Theorem 4.2 shows that the runtime required for an error of size  $\|q - \mathcal{S}_L(q)\|_{L^2(\Gamma)} \leq \epsilon$  is asymptotically bounded by  $\epsilon^{-3/2}$ . Observe in particular that the exponent is independent of the number of bumps  $n$ , whereas straightforward approximation would require the work  $\epsilon^{-n-3/2}$ .

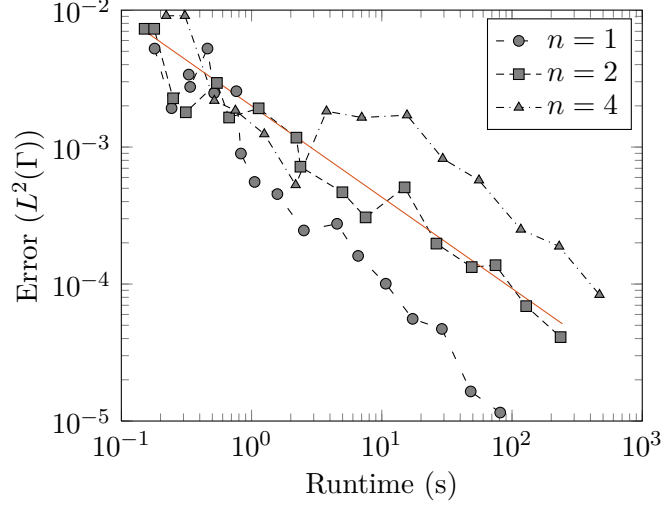
Figure 2 below shows convergence plots for  $n \in \{1, 2, 4\}$ , which exhibit the expected rate of convergence. The runtimes include the solution of the linear systems required for kernel-based approximation. Even though the associated work is not asymptotically negligible for the given work and convergence parameters, this did not affect the results in the ranges of  $L$  we considered. For each  $n \in \{1, 2, 4\}$ , a reference solution was computed with Smolyak's algorithm using  $L_{\max} \gg 1$  and the  $L^2(\Gamma)$ -distance to the results of Smolyak's algorithm with  $n+1 \leq L < L_{\max}$  was approximated using  $10^4$  random evaluations.

## 5.2 Optimization under uncertainty

We consider an advection-diffusion problem with a deterministic source term  $f$ , user-controlled velocity  $z \in B_1(0) \subset \mathbb{R}^2$ , and random diffusion coefficient  $a_m := 1 + \exp(-m)$ , where  $m \sim \mathcal{N}(0, k)$  is a centered Gaussian random field on  $[0, 1]^2$  with covariance  $k(x, y) = \exp(-(10|x - y|)^2)$ . We are



**Figure 1:** Domain of the numerical example in Section 5.1 and domains  $\Gamma^{(j)}$  of the centers  $c_j$ ,  $j \in \{1, \dots, n\}$ .



**Figure 2:** Convergence of Smolyak's algorithm for response surface reconstruction. Expected slope:  $-2/3$  (red).

interested in the spatial average  $Q(u_{(z,m)}) := \int_{(0,1)^2} u_{(z,m)}$  of the solution of

$$\begin{aligned} -\nabla \cdot (a_m \nabla u_{(z,m)}) &= -z \cdot \nabla u_{(z,m)} + f && \text{in } (0,1)^2 \\ \partial_{\mathbf{n}} \nabla u_{(z,m)} + u_{(z,m)} &= u_b && \text{on } \partial(0,1)^2 \end{aligned}$$

where

$$u_b := \begin{cases} 1 & \text{on } \{0\} \times [0,1] \\ 0 & \text{on } \{1\} \times [0,1] \\ \frac{1+\cos(\pi x_1)}{2} & \text{on } [0,1] \times \{0\} \\ \exp(1 - 1/(1-x_1)) & \text{on } [0,1] \times \{1\}. \end{cases}$$

and  $f(x) := 20 \exp(-|x - (0.5, 0.5)|^2)$ .

Our goal is to minimize the expected value of the spatial average plus a quadratic penalty term for large velocities,

$$\min_{z \in B_1(0)} \phi(z),$$

where

$$\phi(z) := v(z) + \psi(z) := E[Q(u_{(z,m)})] + \frac{|z|^2}{10}.$$

For our numerical experiments, we used kernel-based approximations  $S_N : H^4(B_1(0)) \rightarrow L^\infty(B_1(0))$  based on evaluations in  $Y_N \subset B_1(0)$  with  $h_{Y_N, B_1(0)} \lesssim_N N^{-1/2}$ , satisfying

$$\|S_N - \text{Id}\|_{H^4(B_1(0)) \rightarrow L^\infty(B_1(0))} \lesssim_N h_{Y_N, B_1(0)}^3 \lesssim_N N^{-3/2}. \quad (41)$$

Furthermore, we used finite element approximations of  $u_{(z,m)}$  with maximal element size  $h_{\max}$  and  $M \approx h_{\max}^{-2}$  mesh points. The finite element approximations converged at the rate  $h_{\max}^2 \approx M^{-1}$  and required the computational work  $M^{3/2}$ . Consequentially, we applied Smolyak's algorithm from Theorem 4.3 (using Remark 9) with work parameters  $(1, 1, 3/2)$  and convergence parameters  $(3/2, 1/2, 1)$ .

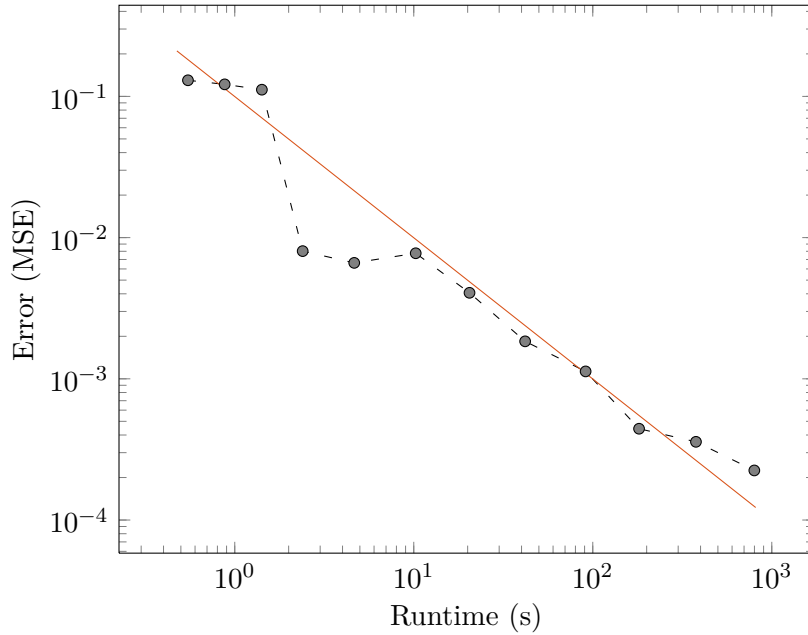
Figure 3 below shows that, as predicted by the theory, the runtime required to achieve the bound

$$E[\|v - \mathcal{S}_L(v)\|_{L^\infty(B_1(0))}^2] \lesssim_\epsilon \epsilon^2, \quad (42)$$

is bounded up to constants by  $\epsilon^{-2}$ , which is an essential improvement on the work  $\epsilon^{-2/3-3/2-2}$  that a straightforward approximation would require for the same bound. A reference solution was computed with Smolyak's algorithm using  $L_{\max} := 15$  and the mean-squared  $L^\infty(B_1(0))$ -distance to the results of Smolyak's algorithm with  $3 \leq L < L_{\max}$  was approximated using  $10^4$  evaluations in  $B_1(0)$  and 20 stochastic repetitions.

Using the surrogate model obtained by Smolyak's algorithm with  $L = 15$ , we obtain the optimal velocity  $z^* \approx (-0.451, -0.062)$  with  $v(z^*) \approx 5.038$  and  $\phi(z^*) \approx 5.059$ .

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**Figure 3:** Convergence of Smolyak's algorithm for optimization under uncertainty. Expected slope:  $-1/2$  (red).

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